

Correlations and fluctuations of matrix elements and cross sections

Bruno Eckhardt, Imre Varga and Péter Pollner ^{a *}

^aFachbereich Physik, Philipps-Universität Marburg,
Renthof 6, D-35032 Marburg an der Lahn, Germany

Abstract

The fluctuations and correlations of matrix elements of cross sections are investigated in open systems that are chaotic in the classical limit. The form of the correlation functions is discussed within a statistical analysis and tested in calculations for a damped quantum kicked rotator. We briefly comment on the modifications expected for systems with slowly decaying correlations, a typical feature in mixed phase spaces.

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1. Introduction

The photo-dissociation cross section as determined by Fermi's golden rule contains a combination of final density of states and transitional matrix elements. The statistical properties of this cross section in a situation of a chaotic dynamics will thus be determined by the statistical properties of both the density of states and the matrix elements. Moreover, if there is a classical underlying dynamics, both will be connected, in a suitable semiclassical limit, to the properties of the classical dynamics. Our aim here is to present a few numerical and theoretical considerations connected to these observations.

We focus on the form of the correlation function of photo-absorption cross sections. Using a random matrix theory approach Alhassid and Fyodorov [1] found a correlation function that consisted of a Lorentzian and a derivative of a Lorentzian with respect to the width. The first term is familiar from the analysis of Ericsson fluctuations in nuclear physics [2,3] and the second one from the correlation function of the Wigner

time delay [4]. The form of the correlation function can now be made plausible if within a statistical model for the cross section the fluctuations in the density of states and in the transition matrix elements are independent, as discussed in section 2.

A semiclassical analysis of this correlation function [5] shows that the relative weight of the two contributions depends on the ratio of the fluctuations of the observable to the mean. In case of a single initial state, random matrix theory fixes this ratio to universal numbers. However, in situations an incoherent superposition of initial states contributes to the cross section, variations in the relative weight are possible. This is illustrated within a numerical analysis for a damped kicked rotator in section 3.

The semiclassical connection also suggests certain modifications in the correlation functions if the classical decay is not purely exponential[6]. In particular, in situations with mixed phase space an algebraic decay is expected[7]. The modifications in the correlation functions include a slower decay and the formation of a cusp at the origin, depending on the exponent of the decay law. In section 4 we propose a model for the form factor and analyze some of the consequences.

We conclude with a brief summary in section 5.

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2. Matrix element correlations within random matrix theory

The quantity we focus on is the density of states weighted by the matrix elements of the observable,

$$\rho_A(E) = \sum_{\mu} A_{\mu} \delta_{\eta}(E - E_{\mu}), \quad (1)$$

where the sum runs over the eigenstates of the system having eigenvalues E_{μ} . The photo-absorption cross section is proportional to this expression if the observable A contains the projection onto the initial state and the dipole operator. The expectation value of \hat{A} can be written as $A_{\mu} = \bar{A} + \delta A_{\mu}$, where \bar{A} is the mean and δA_{μ} is the random fluctuation around its mean. Statistically we assume

$$\langle \delta A_n \rangle = 0, \quad \text{and} \quad \langle \delta A_n \delta A_m \rangle = \sigma_A^2 \delta_{n,m}. \quad (2)$$

The function $\delta_{\eta}(x)$ is a Lorentzian function with half width parameter η , normalized so that as $\eta \rightarrow 0$ it approaches a Dirac- δ . We take the same value of η for all the eigenstates implying a uniform damping. The mean density of states is simply

$$\bar{\rho}_A = \langle \rho_A(E) \rangle_E = \int_B \frac{dE}{B} \rho_A(E) = \frac{N\bar{A}}{B}, \quad (3)$$

where N is the number of levels and B is the energy width of the subset of the spectrum, over which the average $\langle \dots \rangle_E$ is calculated.

The normalized autocorrelation function of the fluctuations of the density of states, $\delta\rho_A(E) = \rho_A(E) - \bar{\rho}_A$ is defined as

$$C(\varepsilon) = \frac{\langle \delta\rho_A(E + \varepsilon) \delta\rho_A(E) \rangle_E}{\bar{\rho}_A^2} \quad (4)$$

$$= \left(\frac{B}{N\bar{A}} \right)^2 \int_B \frac{dE}{B} \rho_A(E + \varepsilon) \rho_A(E) - 1.$$

Inserting the definition (1) in (4) we obtain

$$C(\varepsilon) = \left(\frac{B}{N\bar{A}} \right)^2 \sum_{\mu, \nu} [\bar{A}^2 + \bar{A}(\delta A_{\mu} + \delta A_{\nu}) + \delta A_{\mu} \delta A_{\nu}] g_{\eta}(\varepsilon, E_{\mu}, E_{\nu}) - 1, \quad (5)$$

where we have inserted the shorthand notation

$$g_{\eta}(\varepsilon, E_{\mu}, E_{\nu}) = \langle \delta_{\eta}(E - E_{\mu} + \varepsilon) \delta_{\eta}(E - E_{\nu}) \rangle_E. \quad (6)$$

With the assumption that matrix elements and resonances are uncorrelated [8], averaging over the δA 's eliminates two terms,

$$C(\varepsilon) = \left(\frac{B}{N} \right)^2 \sum_{\mu, \nu} g_{\eta}(\varepsilon, E_{\mu}, E_{\nu}) - 1 \quad (7)$$

$$+ \left(\frac{B}{N\bar{A}} \right)^2 \sum_{\mu, \nu} \langle \delta A_{\mu} \delta A_{\nu} \rangle g_{\eta}(\varepsilon, E_{\mu}, E_{\nu}).$$

In the second term we will utilize (2). Also we will split the first double sum in diagonal ($\mu = \nu$) and non-diagonal ($\mu \neq \nu$) parts. For sufficiently small η the diagonal term is the autocorrelation function of Lorentzian that also yields a Lorentzian.

$$C(\varepsilon) = \left(1 + \frac{\sigma_A^2}{\bar{A}^2} \right) \frac{B^2}{N} \langle \delta_{\eta}(E - \varepsilon) \delta_{\eta}(E) \rangle_E - 1$$

$$+ \left(\frac{B}{N} \right)^2 \sum_{\mu \neq \nu} g_{\eta}(\varepsilon, E_{\mu}, E_{\nu}). \quad (8)$$

After performing the averaging in the first term and in the sum together with the definition in (6), one arrives at

$$C(\varepsilon) = \Delta \frac{\sigma_A^2}{\bar{A}^2} \delta_{2\eta}(\varepsilon) - 1$$

$$+ \Delta \frac{1}{N} \sum_{\mu \neq \nu} \delta_{2\eta}[\varepsilon - (E_{\mu} - E_{\nu})], \quad (9)$$

where $\Delta = B/N$. In the sum one can recognize the appearance of the two-level correlation function in the limit of $\eta \rightarrow 0$. For strongly overlapping resonances, i.e. when $\eta \gg \Delta$ the above expression reduces to

$$C(\varepsilon) \propto \left(\frac{\sigma_A^2}{\bar{A}^2} \frac{\eta}{\eta^2 + \varepsilon^2} + \frac{1}{2\pi} \frac{\eta^2 - \varepsilon^2}{(\eta^2 + \varepsilon^2)^2} \right) \quad (10)$$

Thus the correlation function is characterized by two terms, a Lorentzian and a derivative of a Lorentzian with respect to the broadening parameter η . The weight of the first term comes from the fluctuations of the observable A . In the case when $\hat{A} = |i\rangle\langle i|$ is a projection on the basis state $|i\rangle$. This quantity in random matrix theory (RMT) [9] is $(\beta + 2)/\beta$, where $\beta = 1, 2$, and 4 for the different universality classes the system belongs to (orthogonal, unitary, and symplectic,

respectively). Hence we recover the correlation function derived in Ref. [1] for channels with uniform resonance width.

However, if \bar{A} vanishes, the normalization by \bar{A} is not possible and the second term, which comes from the correlation function of the density of states, cf. (5) and (6), disappears and the correlation function becomes a pure Lorentzian. These findings are thus in accordance with what has been argued on the basis of semiclassical periodic orbit theory[5].

3. Correlations in the quantum kicked rotator

To illustrate the above calculations we calculate the correlation function of the matrix element weighted density of states for a damped kicked rotator.

We consider the statistical properties of observables that are projections onto a subset of the basis states

$$\hat{A} = \sum_{n \in I(m)} |n\rangle\langle n|, \quad (11)$$

where $I(m)$ is a subset of size $m < N$ of the basis set. The fluctuations of the matrix elements $\langle \mu | \hat{A} | \mu \rangle$ over the eigenstates μ of the system describe the cross section fluctuations of the excitation of the system from an initial state $I(m)$ to the final state μ [1,10,11,5]. A possible dipole operator has been absorbed into the definition of $|\mu\rangle$.

The model system we considered is a quantum kicked rotator with a kicking potential

$$V(\phi) = k(\cos \phi - \sin 2\phi). \quad (12)$$

It is known [3,6] that this model belongs to the unitary universality class since the second term in the potential breaks the conjugation symmetry.

We have diagonalized the unitary one-step evolution operator U at a value of the classical kicking strength, K , where complete ergodicity was expected ($K = 7$ [12]). The size of the system was fixed to $N = 201$. The matrix element weighted density of states was defined as

$$\rho_A(\phi) = \sum_{\mu} \langle \mu | \hat{A} | \mu \rangle \left(1 - e^{i(\phi - \phi_{\mu}) - \Gamma/2} \right)^{-1}. \quad (13)$$

The mean value of this observable is simply $\bar{A} = m/N$ where $1 \leq m \leq N$ is the number of states contributing in the projection. We have calcu-

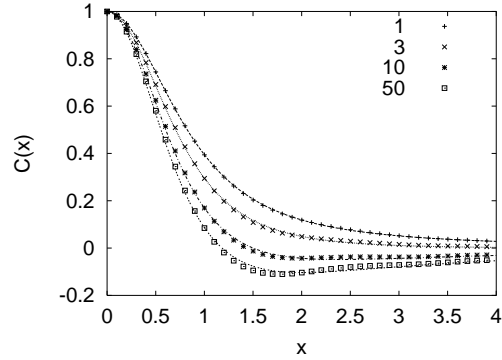


Figure 1. The correlation function $C(x)$ as a function of the eigenvalue separation in units of mean level spacing. The data points are obtained for observables of projections over m basis states indicated in the legend. The continuous curves are fits of the form (15) fitting α and γ independently. The width of the resonances was uniform throughout the spectrum: $\Gamma = \Delta$.

lated the correlation function (4) applied for our case

$$C(x) = \langle \delta \rho_A(\phi + x) \delta \rho_A(\phi) \rangle_{\phi}, \quad (14)$$

i.e. averaging $\langle \dots \rangle_{\phi}$ is done over the eigenphase spectrum extending over $B = 2\pi$. The variables ϕ and x are measured in units of the mean level spacing $\Delta = B/N$ therefore $\bar{\rho}_A = 2\pi\bar{A}/N$. The arguments of [5] and the RMT arguments of the previous section shows, that the correlation function is composed of a Lorentzian and a derivative of a Lorentzian

$$C(x) \propto \left(\alpha \frac{\gamma}{\gamma^2 + x^2} + \frac{1}{2\pi} \frac{\gamma^2 - x^2}{(\gamma^2 + x^2)^2} \right). \quad (15)$$

In (15) $\alpha = \sigma_A^2 / (\bar{A}^2 T_H)$, with the Heisenberg time $T_H = N$. The width γ should come out to be the damping η of (10), in appropriate units.

This expression can be compared to numerical results on the kicked rotator. In Fig. 1 we plot the correlation function obtained for observables that

are projections extending over $m = 1, 3, 10, 50$ basis states. The continuous curves in the figure are fits of the form (15) allowing the two parameters α and γ to vary. The classical estimate for α is [5,6]

$$\alpha = \frac{\sigma_A^2}{\bar{A}^2 N} = \frac{1 - \bar{A}}{\bar{A} N} \propto \frac{1}{m} \quad (16)$$

The variance σ_A^2 follows its classical value for low values of $p = \bar{A} = m/N$ [6]. We obtained a fitted value of $\gamma = 1.11 \Gamma$ (instead of Γ) independent of m and $\alpha = 0.284, 0.135, 0.042$, and 0.009 for $m = 1, 3, 10$, and 50 , respectively. The dependence on m is close to the one predicted by (16) at least for $m > 1$.

4. Open systems and slowly decaying correlations

The correlations described in the previous sections can be derived also using the following phenomenological procedure[1]. The two-level correlation function of a closed chaotic system, $C_0(\varepsilon)$, consists of a Dirac- δ at the origin and a smooth function decreasing to zero for large level separations. This is the Fourier transform of the form factor $K_0(\tau)$. From now on for sake of simplicity we restrict ourselves to the unitary universality class, i.e. we write the RMT form factor in its standard form [9], $K_0(\tau) = 1 - b(\tau)$, with

$$b(\tau) = (1 - |\tau|)\Theta(1 - |\tau|) \quad (17)$$

where $\Theta(x)$ is the step-function. Time τ is measured in units of the Heisenberg time T_H , therefore energy separation ε , in units of mean level spacing Δ . According to RMT the correlation function is

$$\begin{aligned} C_0(\varepsilon) &= \int_{-\infty}^{\infty} d\tau K_0(\tau) \cos(2\pi\varepsilon\tau) \\ &= \delta(\varepsilon) - \left[\frac{\sin(\pi\varepsilon)}{\pi\varepsilon} \right]^2. \end{aligned} \quad (18)$$

Uniform damping, i.e. opening up the system, can be introduced by multiplying the form factor with an exponential decay.

$$K(\tau) = K_0(\tau)e^{-\Gamma|\tau|}, \quad (19)$$

where Γ measures the relaxation rate in units of the Heisenberg time. In fact $\Gamma = T_c/T_H$, where T_c is the relaxation time. When $\Gamma < 1$ ($\Gamma > 1$) the relaxation happens over a time scale longer (shorter) than T_H , hence produces correlations over energy scales lower than (beyond) mean level spacing. The resulting form factor for different values of $\Gamma = 0.0, 0.1, 1.0$ and 5.0 are plotted in Fig. 2. The Fourier transform of (19) results in

$$C(\varepsilon) = C_1(\varepsilon) + C_2(\varepsilon) \quad (20)$$

where

$$C_1(\varepsilon) = \int_{-\infty}^{\infty} d\tau e^{-\Gamma|\tau|} \cos(2\pi\varepsilon\tau), \quad (21)$$

$$C_2(\varepsilon) = - \int_{-1}^1 d\tau (1 - |\tau|) e^{-\Gamma|\tau|} \cos(2\pi\varepsilon\tau). \quad (22)$$

The first term $C_1(\varepsilon)$ is a Lorentzian from the broadening of the δ -function and the second term, the convolution of the Lorentzian with the two-level cluster function, leads, in the limit of large Γ , to the derivative of the Lorentzian. The corresponding correlation functions $C(\varepsilon)$ are plotted in Fig. 3.

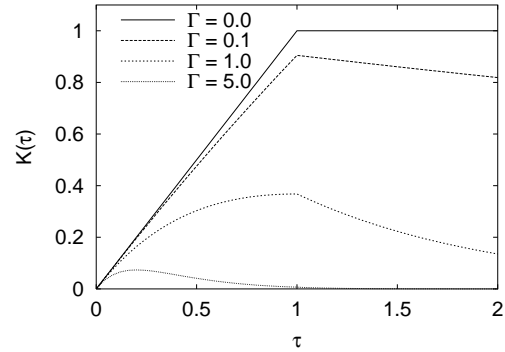


Figure 2. The form factor for different uniform damping constants $\Gamma = 0.0, 0.1, 1.0$, and 5.0 .

These considerations led us to extend the above approach in another direction. Let us assume that the quantum return probability, the form factor, is damped slower than exponential, i.e. in an algebraic fashion. The correlation function in this case will contain signatures of the slowing

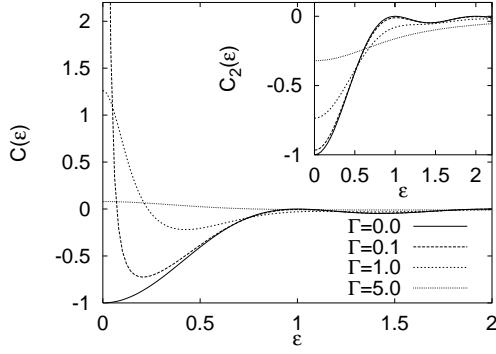


Figure 3. The correlation function, $C(\varepsilon)$ (see Eq. (20)), of an open system for different uniform damping rates $\Gamma = 0.0, 0.1, 1.0$, and 5.0 . The inset shows $C_2(\varepsilon)$ (22).

down of the classical dynamics, a behavior that is expected to be prominent in systems with mixed phase space [13].

Such an algebraic damping may be introduced in the phenomenological ansatz

$$K(\tau) = K_0(\tau) (1 + c\tau)^{-a}, \quad (23)$$

where $c = T_H/T_c$ is the ratio of the decorrelation time T_c compared to the Heisenberg time T_H . As in the case of exponential damping, for $c < 1$ ($c > 1$) the slow decorrelation of classical trajectories due to the presence of the hierarchy of stable islands [13,14] occur on a time scale that is longer (shorter) than the Heisenberg time that produces correlations over energy scales lower than (beyond) mean level spacing. By fixing one of the parameters a and c the variation of the other results in changes in different parts of the correlation function. Similarly as in (20) we find

$$C(\varepsilon) = C_1(\varepsilon) + C_2(\varepsilon) \quad (24)$$

where

$$C_1(\varepsilon) = \int_{-\infty}^{\infty} d\tau \frac{\cos(2\pi\varepsilon\tau)}{(1 + c|\tau|)^a}, \quad (25)$$

$$C_2(\varepsilon) = - \int_{-1}^1 d\tau \frac{1 - |\tau|}{(1 + c|\tau|)^a} \cos(2\pi\varepsilon\tau). \quad (26)$$

We have plotted the correlation function for the case when $a = 4/3$. This type of correlations can

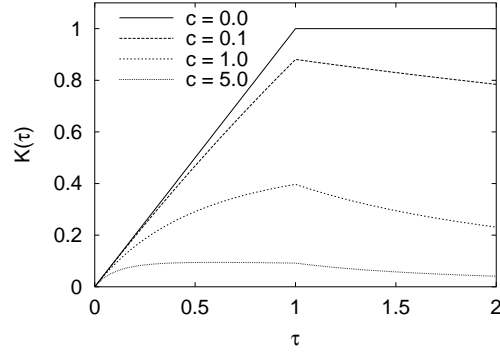


Figure 4. The form factor with algebraic damping ($a = 4/3$) for different ratios of the Heisenberg time T_H compared to the decorrelation time T_c , $c = T_H/T_c = 0.0, 0.1, 1.0$, and 5.0 .

be expected to occur in systems with mixed phase space [14]. In Fig. 5 the curves demonstrate that a low value of c results in only a slight modification of the correlations while large c , i.e. when $T_c < T_H$ the algebraic decorrelation results in changes both in the $\varepsilon < 1$ and $\varepsilon > 1$ regimes. This is in contrast to previous expectations [14] that the dynamics occurring over time scales up to T_H should show up in the correlation function on energy scales beyond mean level spacing only.

To show the similarities and differences between correlation functions obtained for exponential and power law damping we plot the value at $\varepsilon = 0$, i.e. the variance of the fluctuating observable under investigation. In Fig. 6 we can see that for $T_c > T_H$ the two types of damping functions yield the same correlation time dependence, $\propto (T_H/T_c)^{-1}$. In the case of $T_c < T_H$ the exponential damping produces a $(T_H/T_c)^{-2}$ dependence and the power law version a $(T_H/T_c)^{-a}$ (in the case shown $a = 4/3$).

An even more striking difference between the fast and slow decorrelations shows up in the low- ε behavior of the correlation function. As pointed out already by Lai *et al.* [15] non-hyperbolic systems produce a cusp in the correlation function

$$C(\varepsilon) \sim C(0) - C_a \varepsilon^{a-1} \quad (27)$$

where $C_a = b_a c^{-(a-1)}$ is a positive constant and a is the exponent of the classical return probability $P(t) \sim t^{-a}$. This behavior is to be contrasted

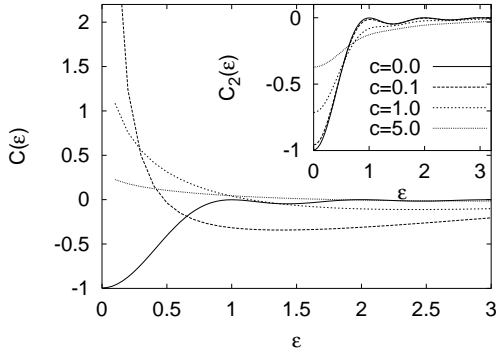


Figure 5. The correlation function, $C(\varepsilon)$, of a system containing algebraic decorrelation with exponent $a = 4/3$ (see Eq. (24)). The curves stand for different ratios of the Heisenberg time T_H compared to the decorrelation time T_c , $c = T_H/T_c$, with $c = 0.0, 0.1, 1.0$, and 5.0 . The inset shows $C_2(\varepsilon)$ (26).

with the hyperbolic case when the low- ε behavior is expected to be

$$C(\varepsilon) \sim C(0) - C_2\varepsilon^2, \quad (28)$$

where $C_2 \sim \Gamma^{-2}$ is a constant depending on the exponential relaxation rate. In Fig. 7 we show the cusp at low- ε in the case of power law decorrelation and the parabolic behavior for exponential damping. The curves represent especially the cases when $T_H/T_c \geq 1$, i.e. when the classical correlations appear at time scales below the Heisenberg time. In this case one expects deviations at $\varepsilon \geq 1$. The cusp at low- ε , however, is present for any value of c .

We would like to emphasize that the apparent contradiction between the behavior of the correlation function for power law decorrelation (27) and that of refs. [13,14] resides probably in the difference of the classical return probability functions considered. We took the modification of the RMT form factor (23) while in refs. [13,14] the classical return probability of $P(t) \sim t^z$ was used.

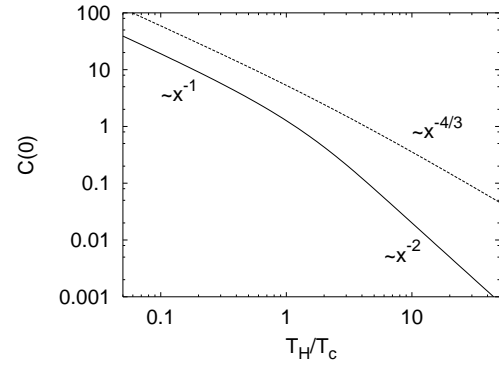


Figure 6. The value of $C(\varepsilon)$ at $\varepsilon = 0$ for exponential (continuous) and power law damping (dashed curve). The ratio T_H/T_c is Γ for exponential and c for power law damping. The power law curve was obtained for the exponent of $a = 4/3$.

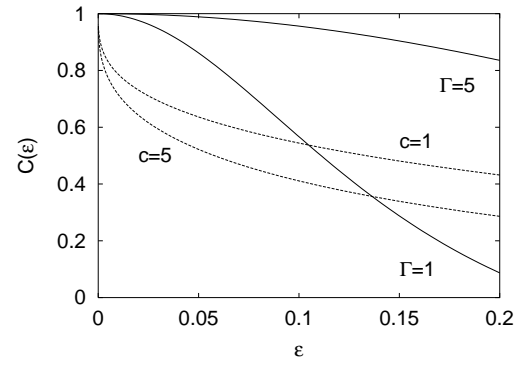


Figure 7. The correlation function for low- ε for exponential (continuous) and power law damping (dashed curve) for two different values of the decorrelation time $T_c/T_H = 1$, and 5 . The power law curve was obtained for the exponent of $a = 4/3$.

5. Final remarks

The variations in the correlation functions for the different situations are not very large and perhaps difficult to detect. This seems to apply in particular to cases with an algebraic decay, especially in view of the fact that the exponents are not universal and might be clouded by a distribution of algebraic decay laws. The modifications due to variations in matrix elements and thus a stronger emphasis of the derivative part of the correlation function could perhaps be achieved in

incoherent superpositions of cross sections from different initial states. Analysis of experimental data in this direction seems worthwhile.

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